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Numerical Modelling of Optical Trapping

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Optical trapping is a widely used technique, with many important applications in biology and metrology. Complete modelling of trapping requires calculation of optical forces, primarily a scattering problem, and non-optical forces. The T-matrix method is used to calculate forces acting on spheroidal and cylindrical particles.
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1. Introduction

Optical trapping provide three-dimensional confinement and manipulation of microscopic particles by a focussed laser beam. Optical trapping is a powerful and widespread technique, with the single-beam gradient trap (also known as optical tweezers) in use for a large number of biological and other applications.
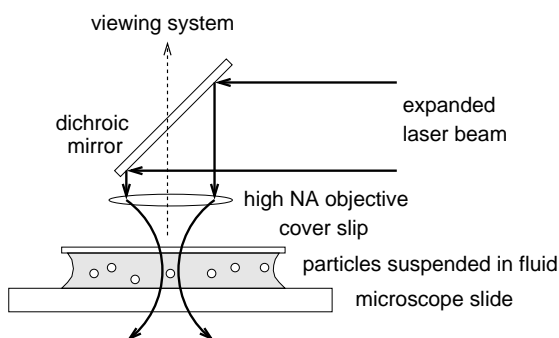

Figure 1. Schematic diagram of a typical optical tweezers setup

The trapping beam applies optical forces (usually divided into a gradient force, acting towards areas of higher irradiance, and scattering forces, including absorption and reflection forces) to the particle.

The optical forces and torques result from the transfer of momentum and angular momentum from the trapping beam to the particle. Various approximate methods such as geometric optics or Rayleigh approximations are often used for the calculation of the optical forces. Such approximate methods are not necessary, since electromagnetic scattering theory can be used for the calculation of forces, avoiding the limited ranges of applicability of the approximate methods.

Other forces will also affect the motion of the particle. The most important of these forces, gravity, buoyancy, and viscous drag as the particle moves through the surrounding fluid, are readily taken into account in the theory presented here.

2. Trapping as a scattering problem

The optical forces and torques applied to the particle result from the transfer of momentum and angular momentum from the trapping beam to the particle. The total momentum transfer can be found by solving the electromagnetic scattering problem. A variety of numerical methods can be used – finite element method (FEM), finite difference time domain method (FDTD), discrete dipole approximation (DDA) [1], the T-matrix method [2,3], etc.

A number of these have been used for optical force calculations, including forces in optical

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traps [4,5]. One method, however, stands out as ideal for trapping force calculations – the T-matrix method. The T-matrix method can be considered an extension of Mie theory to arbitrarily shaped particles with arbitrary illumination. The main advantage of the T-matrix method is that trapping calculations usually involve repeated calculation of the scattering for the same particle under differing illumination. In this case, the T-matrix needs only be calculated once, since it is independent of the fields, whereas methods such as FEM, FDTD and DDA will require the entire calculation to be repeated.

In the T-matrix method, the incident trapping field illuminating the particle is expressed as a sum of regular vector spherical wave functions (VSWFs):

$$\mathbf{E}_{\mathrm{inc}}(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [a_{mn}\mathbf{RgM}_{mn}(k\mathbf{r}) + b_{mn}\mathbf{RgN}_{mn}(k\mathbf{r})] \qquad (1)$$

where

$$\mathbf{RgM}_{mn}(k\mathbf{r}) = (-1)^m d_n \exp(im\phi) \times j_n(kr)\mathbf{C}_{mn}(\theta), \qquad (2)$$

$$\mathbf{RgN}_{mn}(k\mathbf{r}) = (-1)^m d_n \exp(im\phi) \times \left\{ \frac{n(n+1)}{kr} j_n(kr)\mathbf{P}_{mn}(\theta) + \left[j_{n-1}(kr) - \frac{n}{kr}j_n(kr) \right] \mathbf{B}_{mn}(\theta) \right\}, \qquad (3)$$

$$\mathbf{B}_{mn}(\theta) = \hat{\theta}\frac{d}{d\theta}d_{0m}^n(\theta) + \hat{\phi}\frac{im}{\sin\theta}d_{0m}^n(\theta), \qquad (4)$$

$$\mathbf{C}_{mn}(\theta) = \hat{\theta}\frac{im}{\sin\theta}d_{0m}^n(\theta) - \hat{\phi}\frac{d}{d\theta}d_{0m}^n(\theta), \qquad (5)$$

$$\mathbf{P}_{mn}(\theta) = \hat{r}d_{0m}^n(\theta), \qquad (6)$$

$$d_n = \left(\frac{2n+1}{4\pi n(n+1)} \right)^{\frac{1}{2}}, \qquad (7)$$

$j_n(kr)$ are spherical Bessel functions, and $d_{0m}^n(\theta)$ are Wigner d functions.

Similarly, the scattered fields are expressed as a VSWF expansion. In this case, since the far field must be an outgoing radiation field,

$$\mathbf{E}_{\mathrm{scat}}(\mathbf{r}) = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [p_{mn}\mathbf{M}_{mn}(k\mathbf{r}) + q_{mn}\mathbf{N}_{mn}(k\mathbf{r})] \qquad (8)$$

where $\mathbf{M}_{mn}(k\mathbf{r})$ and $\mathbf{N}_{mn}(k\mathbf{r})$ are the same as $\mathbf{RgM}_{mn}(k\mathbf{r})$ and $\mathbf{RgN}_{mn}(k\mathbf{r})$, with the spherical Bessel functions replaced by spherical Hankel functions of the first kind, $h_n^{(1)}(kr)$.

From the linearity of the Maxwell equations, there is a linear relationship between the incident and scattered fields:

$$p_{mn} = \sum_{m'n'} T_{mnm'n'}^{(11)}a_{m'n'} + T_{mnm'n'}^{(12)}b_{m'n'} \qquad (9)$$

$$q_{mn} = \sum_{m'n'} T_{mnm'n'}^{(21)}a_{m'n'} + T_{mnm'n'}^{(22)}b_{m'n'} \qquad (10)$$

The T-matrix can be calculated using the extended boundary condition method (EBCM) [2, 3]. For spherical particles, the T-matrix becomes diagonal, and the non-zero elements are the usual Mie coefficients. For rotationally symmetric particles, the T-matrix is diagonal with respect to n. Computer codes to calculate T-matrices for such rotationally symmetric particles are available [6].

3. Representation of the trapping beam

The use of the T-matrix method for scattering calculations requires that the trapping beam be represented in terms of vector spherical wave functions, that is, the coefficients a_{mn} and b_{mn} in equation (1) need to be found. The regular VSWFs $\mathbf{RgM}_{mn}$ and $\mathbf{RgN}_{mn}$ provide a complete set of modes or partial waves, each individually satisfying the Maxwell equations, which can be used to represent any incident electromagnetic wave. For the simple case of a plane wave, $\mathbf{E}(\mathbf{r}) = \mathbf{E}_0 \exp(i\mathbf{k} \cdot \mathbf{r})$, with $\mathbf{k}$ in the direction (θ, ϕ), the expansion coefficients are [2,3]

$$a_{mn} = 4\pi(-1)^m i^n d_n \mathbf{C}_{mn}^{\star} \cdot \mathbf{E}_0 \exp(-im\phi) \qquad (11)$$

$$b_{mn} = 4\pi(-1)^m i^{n-1} d_n \mathbf{B}_{mn}^{\star} \cdot \mathbf{E}_0 \exp(-im\phi). \qquad (12)$$

Note that the amplitude vector $\mathbf{E}_0$ contains the information regarding the polarisation and phase of the wave, and can be complex.

In an optical trap, the incident field is usually a strongly focussed Gaussian or other beam. In principle, such a beam can either be decomposed directly into a VSWF representation, or into a plane wave spectrum, from which the VSWF expansion coefficients can be found using equations (11) and (12). In practice, this is problematic, since the usual descriptions of beams do not actually satisfy the Maxwell equations.

For the case of Gaussian beams, either plane wave expansion [7] or direct VSWF expansion [8, 9] can be used, although neither will give a beam identical to a paraxial or Davis Gaussian beam.

4. Optical forces

Using the T-matrix method, with the T-matrix calculated by the publicly available code by Mishchenko [6], and the beam shape coefficients in the localised approximation by Gouesbet [8,9] used to describe the beam, we calculated the variation of the axial force acting on particles of varying shape as a function of their position along the beam axis.

The particles are polystyrene ($n = 1.59$) prolate spheroids and cylinders, of varying aspect ratio as indicated (see figure 2). The particles are of equal volume, with a volume equal to that of a sphere of radius 0.75μm, and are trapped in water by a Gaussian beam of waist width 0.8μm and free space wavelength 1064nm.
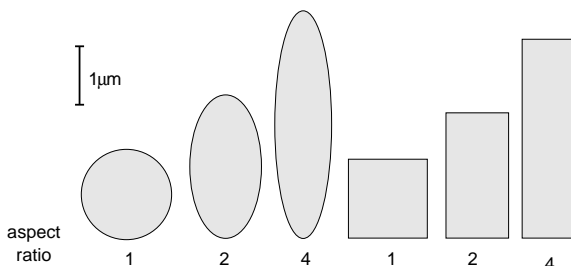
Preliminary results of the axial forces acting on the spheroids and cylinders are shown in figures 3 and 4. A negative position on the beam axis indicates a position before the focal plane is reached, a positive position is after the focus. A positive force acts to push the particle in the direction of propagation of the beam, a negative force will act to axially trap the particle. If only optical forces are acting, the particle will come to rest at the zero optical force position where force curve crosses the zero force line with a negative gradient.
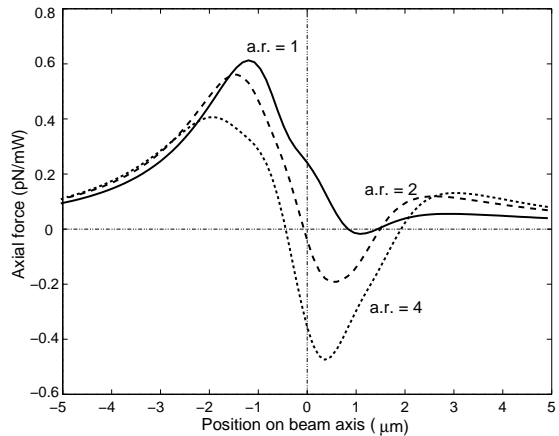

Figure 3. Axial force acting on spheroids of aspect ratios 1, 2, and 4, in pN per milliwatt of total beam power.

The trapping forces acting on the spheroid and cylinder with aspect ratio 1 is very small. This is due to interference due to reflections from the rear surface of the particle [10].

Thorough investigation of the effects of beam shape and particle size and shape will be carried out in the near future. Where possible, the results from this model will be compared with available observations.
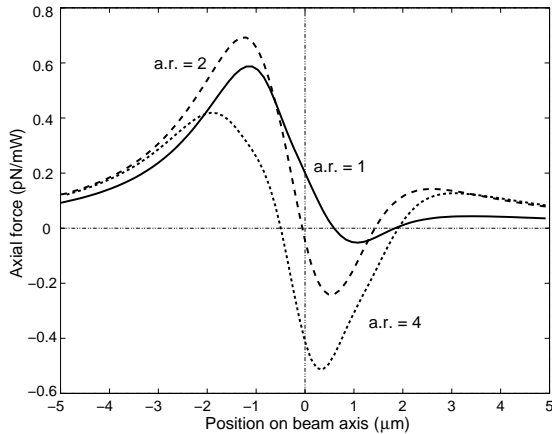

Figure 2. Differently shaped spheroidal and cylindrical particles with aspect ratios of 1, 2, and 4.

Figure 4. Axial force acting on cylinders of aspect ratios 1, 2, and 4, in pN per milliwatt of total beam power.

5. Viscous drag

Motion of the particle through the surrounding fluid results in viscous drag forces, which will be a dominant force on a trapped particle in motion, or in a moving fluid.

The Reynolds numbers of typical motion in trapping are extremely low. For example, if the spherical particle considered previously (see figure 3) is trapped by a 10 mW beam, forces on the order of 5 pN can be applied. The terminal speed can be found from Stokes' Law:

$$D = 6\pi\mu v a \tag{13}$$

where D is the drag force, μ is the viscosity of the surrounding fluid , v is the speed of the sphere, and a is the radius. If the considered sphere is trapped in water ($\mu = 1 \times 10^{-3}$ Ns/m^2 at 20°), the terminal speed will be $\approx 350\mu$m/s. This gives a Reynolds number Re $= \rho v l/\mu = \approx 5 \times 10^{-4}$, showing that perfect laminar flow can be assumed – Stokes' Law is an excellent approximation.

The characteristic time τ at which the terminal speed is approached is the ratio of the mass to the Stokes drag coefficient, so $\tau = m/(6\pi\mu a) \approx 1 \times 10^{-7}$ s, which is independent of the trapping force. For calculating the motion of a trapped particle, we can assume that

$$\dot{\mathbf{r}} \propto \mathbf{F} \tag{14}$$

rather than $\ddot{\mathbf{r}} \propto \mathbf{F}$, since the particle will be moving at very close to the terminal velocity at all times, as long as the time step in the calculation is large compared to τ.

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